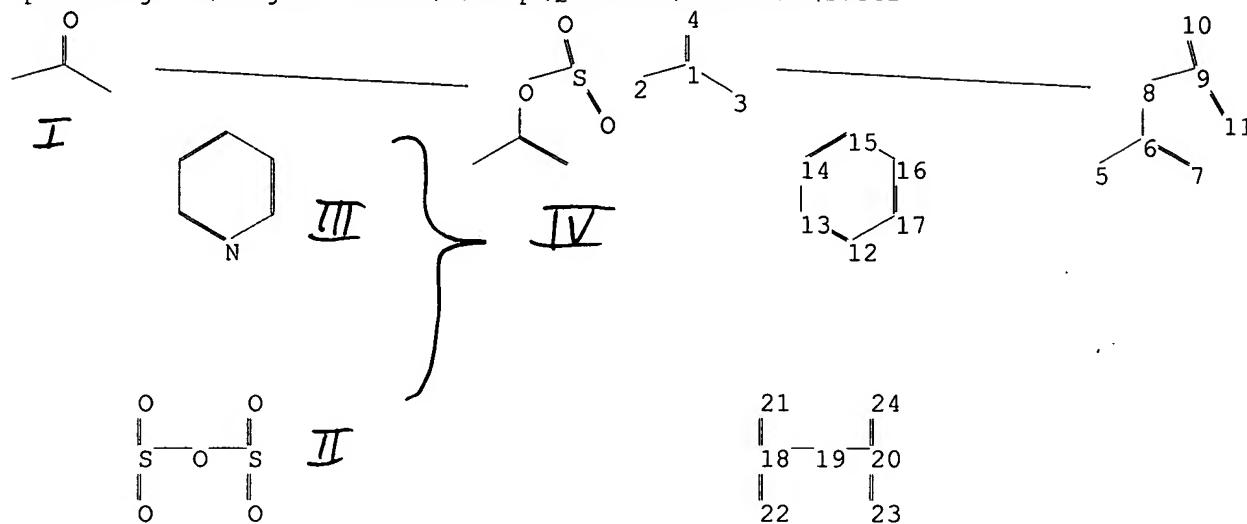


identification.

=>

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chain nodes :

1 2 3 4 5 6 7 8 9 10 11 18 19 20 21 22 23 24

ring nodes :

12 13 14 15 16 17

chain bonds :

1-2 1-3 1-4 5-6 6-7 6-8 8-9 9-10 9-11 18-19 18-21 18-22 19-20 20-23
20-24

ring bonds :

12-13 12-17 13-14 14-15 15-16 16-17

exact/norm bonds :

1-4 6-8 8-9 9-10 9-11 18-19 18-21 18-22 19-20 20-23 20-24

exact bonds :

1-2 1-3 5-6 6-7

normalized bonds :

12-13 12-17 13-14 14-15 15-16 16-17

Match level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS
10:CLASS 11:CLASS 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:CLASS
19:CLASS 20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS

fragments assigned product role:

containing 5

fragments assigned reactant/reagent role:

containing 1

containing 12

containing 18
node mappings:
1:6 4:8 2:5 3:7

L1 STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> d
L1 HAS NO ANSWERS
L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s 11 full
FULL SEARCH INITIATED 13:03:26 FILE 'CASREACT'
SCREENING COMPLETE - 278 REACTIONS TO VERIFY FROM
100.0% DONE 278 VERIFIED 22 HIT RXNS
SEARCH TIME: 00.00.01

52 DOCUMENTS

9 DOCS

L2 9 SEA SSS FUL L1 (22 REACTIONS)

=> d ibib abs hit 1-9

L2 ANSWER 1 OF 9 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 143:7446 CASREACT

TITLE: Synthesis and characterization of cross-conjugated

oligo(phenylene enynylene)s

AUTHOR(S): Cho, Joon; Zhao, Yuming; Tykwienski, Rik R.
Corporate Source: Department of Chemistry, University of Alberta,

Edmonton, AB, T6G 2G2, Can.

SOURCE: ARKIVOC (Gainesville, FL, United States) (2005), (4),

142-150

CODEN: AGFUAR

URL:

http://www.arkat-usa.org/ark/journal/2005/I04_zeff

irov/1369/1369.pdf

PUBLISHER: Arkat USA Inc.

DOCUMENT TYPE: Journal; (online computer file)

LANGUAGE: English

AB The synthesis and characterization of a series of cross-conjugated

oligo(phenylene enynylene)s via the Sonogashira protocol is reported.

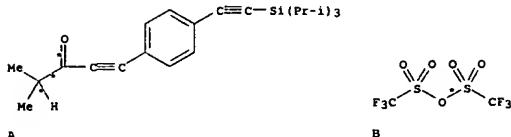
The structural properties of these oligomers have been established by ¹H and ¹³C NMR and IR spectroscopies, as well as mass spectrometry. Their electronic absorption and emission behavior has been investigated via UV/Vis and fluorescence spectroscopy. The results of this study demonstrate that electronic communication along the conjugated framework of these oligomers is limited due to the presence of a cross-conjugated enyne framework and arylene fragments.

REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR

THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

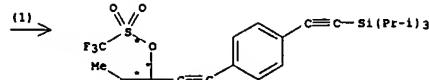
FORMAT

RX(1) OF 28 ...A + B ==> C...



L2 ANSWER 1 OF 9 CASREACT COPYRIGHT 2006 ACS on STN

(Continued)



C YIELD 85%

RX(1) RCT A 852459-84-8, B 358-23-6
 RGT D 38222-83-2 Me-(t-Bu)2-pyridine
 PRO C 852459-83-7
 SOL 75-09-2 CH2Cl2
 CON SUBSTAGE(1) 0 deg C
 SUBSTAGE(2) 0 deg C -> room temperature
 SUBSTAGE(3) 4 hours, room temperature
 NTE Sonogashira coupling

L2 ANSWER 2 OF 9 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 142:279793 CASREACT

TITLE: Synthesis, structure, and nonlinear optical properties of cross-conjugated perphenylated

iso-polydiacetylenes

AUTHOR(S): Zhao, Yuming; Slepkov, Aaron D.; Akoto, Clement Osei; McDonald, Robert; Hegemann, Frank A.; Tykwienski, Rik R.

R. Corporate Source: Department of Chemistry, Memorial University of Newfoundland, St. John's, NL, A1B 3X7, Can.

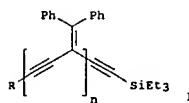
SOURCE: Chemistry--A European Journal (2005), Volume Date 2004, 11(1), 321-329

CODEN: CEUJED; ISSN: 0947-6539

Wiley-VCH Verlag GmbH & Co. KGaA

Journal English

GI



AB Monodisperse, cross-conjugated perphenylated iso-polydiacetylene (iso-PDA)

oligomers I (R = Me3Si, n = 1; R = Et3Si; n = 2, 3, 5, 7, 9, 11, 13, 15) have been synthesized by using a palladium-catalyzed cross-coupling protocol. Structural characteristics elucidated by x-ray crystallography demonstrate a non-planar backbone conformation for the oligomers.

due to the steric interactions between alkylidene Ph groups. The electronic absorption spectra of the oligomers show a slight red-shift of the maximum absorption wavelength as the chain length increases from dimer I (n = 2) to pentadecamer I (n = 15) a trend that has saturated by the stage of nonamer I (n = 9). Fluorescence spectroscopy confirms that the pendent Ph groups present on the oligomer framework enhance emission, and the relative emission intensity consistently increases as a function of chain length

n. The mol. third-order nonlinearities, χ , for this oligomer series have been measured via differential optical Kerr effect (DOKE) detection and show a superlinear increase as a function of the oligomer chain length.

n. Mol. modeling and spectroscopic studies suggest that iso-PDA oligomers

I (n > 7) adopt a coiled, helical conformation in solution

REFERENCE COUNT: 66 THERE ARE 66 CITED REFERENCES AVAILABLE FOR THIS

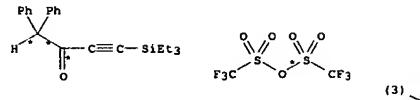
RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L2 ANSWER 2 OF 9 CASREACT COPYRIGHT 2006 ACS on STN

(Continued)

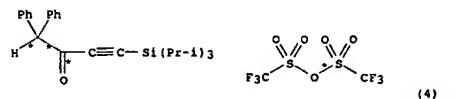
RX(3) OF 125 ...C + H ==> I...



I YIELD 79%

RX(3) RCT C 845725-73-7, H 358-23-6
 RGT J 585-48-8 2,6-Di-t-Bu-pyridine
 PRO I 339577-77-4
 SOL 75-09-2 CH2Cl2
 CON room temperature

RX(4) OF 125 ...G + H ==> K...

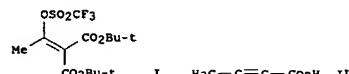


K YIELD 32%

L2 ANSWER 2 OF 9 CASREACT COPYRIGHT 2006 ACS on STN
 RX(4) RCT G 845725-74-8, H 358-23-6
 RGT J 585-48-2, 2,6-Di-t-Bu-pyridine
 PRO K 845725-75-9
 SOL 75-09-2 CH₂Cl₂
 CON room temperature

(Continued)

L2 ANSWER 3 OF 9 CASREACT COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 141:140115 CASREACT
 TITLE: Decarboxylative elimination of enol triflates as a general synthesis of acetylenes
 AUTHOR(S): Fleming, Ian; Ramerao, Chandrashekhar
 CORPORATE SOURCE: Department of Chemistry, Cambridge, CB2 1EW, UK
 SOURCE: Organic & Biomolecular Chemistry (2004), 2(10), 1504-1510
 CODEN: OBRKAK; ISSN: 1477-0520
 PUBLISHER: Royal Society of Chemistry
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI

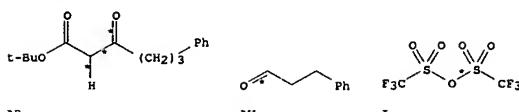


AB The enol trifluoromethanesulfonates of tert-Bu β -keto esters and β -keto esters can be hydrolyzed to the corresponding carboxylic acids by dissolution in trifluoroacetic acid. The dicarboxylic acids undergo mild decarboxylative elimination to give acetylenes in aqueous sodium bicarbonate solution at room temperature. Similarly, monocarboxylic acids give terminal and mid-chain acetylenes by refluxing in acetone with potassium carbonate. One of the substituents on the acetylenes can be Me, primary alkyl, secondary alkyl or ethynyl, and the other can be a carboxylic acid. Hydrogen or primary alkyl, but the enol trifluoromethanesulfonates could not be prepared when one of the substituents was tert-Bu, nor when both substituents on the precursor to the acetylene were secondary alkyl. For example, reaction of trifluoromethanesulfonic acid anhydride with (acetyl)propanedioic acid bis(1,1-dimethylethyl) ester gave a desired enol triflate, 1-[(trifluoromethyl)sulfonyloxy]ethylidene propanedioic acid bis(1,1-dimethylethyl) ester (I). Saponification of I gave the diacid, 1-[(trifluoromethyl)sulfonyloxy]ethylidene propanedioic acid. Decarboxylation of the acid gave 2-butyne-1,4-dioic acid (II).
 REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS

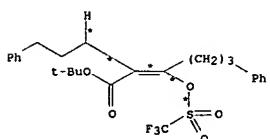
FORMAT RECORD. ALL CITATIONS AVAILABLE IN THE RE

RX(96) OF 118 COMPOSED OF RX(22), RX(26), RX(29)
 RX(96) AR + AW + I ==> BL

L2 ANSWER 3 OF 9 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



3 STEPS
 →



BK
 YIELD 86%

RX(22) RCT AR 235087-26-8, AW 104-53-0

STAGE(1)
 RGT AY 7550-45-0 TiCl₄, AZ 110-86-1 Pyridine
 SOL 109-99-9 THF, 75-09-2 CH₂Cl₂
 CON SUBSTAGE(1) 30 minutes, 0 deg C
 SUBSTAGE(2) 16 hours, room temperature

STAGE(2)
 RGT F 12125-02-9 NH₄Cl
 SOL 7732-18-5 Water
 CON room temperature

PRO AX 725340-58-9
 NTE stereoselective, isomer mix.

RX(26) RCT AX 725340-58-9
 RGT BF 1333-74-0 H₂
 PRO BZ 235087-25-9
 CAT 7440-05-3 Pd
 SOL 67-56-1 MeOH
 CON 24 hours, room temperature

RX(29) RCT BZ 235087-25-9

L2 ANSWER 3 OF 9 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

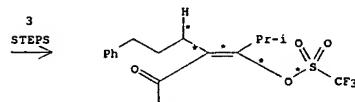
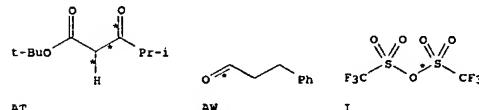
STAGE(1)
 RGT L 7646-69-7 NaH
 SOL 60-29-7 Et₂O
 CON 1 hour, 0 deg C

STAGE(2)
 RGT I 358-23-6
 CON SUBSTAGE(1) 1 hour, 0 deg C
 SUBSTAGE(2) 1 hour, room temperature

STAGE(3)
 RGT F 12125-02-9 NH₄Cl
 SOL 7732-18-5 Water
 CON room temperature

PRO BK 235087-28-2

RX(98) OF 118 COMPOSED OF RX(23), RX(27), RX(30)
 RX(98) AT + AW + I ==> BL



BL
 YIELD 92%

RX(23) RCT AT 94250-54-1, AW 104-53-0

STAGE(1)
 RGT AY 7550-45-0 TiCl₄, AZ 110-86-1 Pyridine
 SOL 109-99-9 THF, 75-09-2 CH₂Cl₂
 CON SUBSTAGE(1) 30 minutes, 0 deg C
 SUBSTAGE(2) 16 hours, room temperature

STAGE(2)
 RGT F 12125-02-9 NH₄Cl
 SOL 7732-18-5 Water
 CON room temperature

L2 ANSWER 3 OF 9 CASREACT COPYRIGHT 2006 ACS on STN
 PRO BA 725340-63-6
 NTE stereoselective, isomer mix.

RX(27) RCT BA 725340-63-6
 RGT BF 1333-74-0 H2
 PRO BI 235087-26-0
 CAT 7440-05-3 Pd
 SOL 67-56-1 MeOH
 CON 24 hours, room temperature

RX(30) RCT BI 235087-26-0

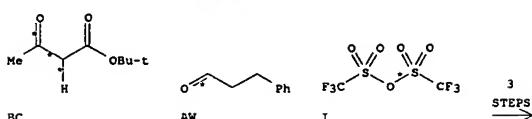
STAGE(1)
 RGT L 7646-69-7 NaH
 SOL 60-29-7 Et2O
 CON 1 hour, 0 deg C

STAGE(2)
 RCT I 358-23-6
 CON SUBSTAGE(1) 1 hour, 0 deg C
 SUBSTAGE(2) 1 hour, room temperature

STAGE(3)
 RGT F 12125-02-9 NH4Cl
 SOL 7732-18-5 Water
 CON room temperature

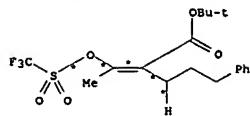
PRO BL 235087-30-6

RX(100) OF 118 COMPOSED OF RX(25), RX(28), RX(31)
 RX(100) BC + AW + I ==> BM



(Continued)

L2 ANSWER 3 OF 9 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



BM
 YIELD 71%

RX(25) RCT BC 1694-31-1, AW 104-53-0

STAGE(1)
 RGT AY 7550-45-0 TiCl4, AZ 110-86-1 Pyridine
 SOL 109-99-9 THF, 75-09-2 CH2Cl2
 CON SUBSTAGE(1) 30 minutes, 0 deg C
 SUBSTAGE(2) 16 hours, room temperature

STAGE(2)
 RGT F 12125-02-9 NH4Cl
 SOL 7732-18-5 Water
 CON room temperature

PRO BD 725340-53-4
 NTE stereoselective, isomer mix.

RX(28) RCT BD 725340-53-4
 RGT BF 1333-74-0 H2
 PRO BJ 725340-75-0
 CAT 7440-05-3 Pd
 SOL 67-56-1 MeOH
 CON 24 hours, room temperature

RX(31) RCT BJ 725340-75-0

STAGE(1)
 RGT L 7646-69-7 NaH
 SOL 60-29-7 Et2O
 CON 1 hour, 0 deg C

STAGE(2)
 RCT I 358-23-6
 CON SUBSTAGE(1) 1 hour, 0 deg C
 SUBSTAGE(2) 1 hour, room temperature

STAGE(3)
 RGT F 12125-02-9 NH4Cl
 SOL 7732-18-5 Water
 CON room temperature

L2 ANSWER 3 OF 9 CASREACT COPYRIGHT 2006 ACS on STN (Continued)
 PRO BM 725340-88-5

L2 ANSWER 4 OF 9 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 140-111001 CASREACT
 TITLE: Fragmentations of (E)- and (Z)-isomers of 2-methylbuten-1-yl(aryl) iodonium triflates:

competing

mechanisms for enol triflate formation

Hinkle, Robert J.; Mikowski, Ann M.

Dep. Chem., The College of William and Mary,

Williamsburg, VA, 23187-8795, USA

SOURCE: ARKIVOC (Gainesville, FL, United States) (2003), (6), 201-212

CODEN: AGFUAR

URL: http://www.arkat-usa.org/journal/2003/Varvogi_is/AV-745A/745A.pdf

PUBLISHER: Arkat USA Inc.

DOCUMENT TYPE: Journal; (online computer file)

LANGUAGE: English

AB We examined fragmentation reactions of (E)- and (Z)-2-methylbuten-1-yl(aryl) iodonium triflates (aryl = C6H5- 4-(CF3)C6H4, 3,5-(CF3)2C6H4-

to afford aryl iodides and six enol triflates. Four of these vinyl triflates involve alkyl migrations followed by triflate trapping of secondary vinyl cations, whereas two do not involve migrations.

Fragmentation rates in dry, neutral CDCl3 were determined as were the distributions of enol triflate products. The ratios of rate constants for the (E)-/(Z)-isomers ranged between 5.0 and 8.5 and, in all salts, the rearranged enol triflate derived from migration of the alkyl moiety

trans- to the aryliodonio- nucleofuge was observed in the greatest quantities.

These data indicate that the fragmentation rates are significantly determined

by the migratory aptitude of the trans- β -alkyl substituent and departure of the aryliodonio-nucleofuge occurs by anachiric assistance. The ratios of inverted "unrearranged" enol triflate products were greater for the (Z)-isomers of the iodonium salt precursors indicating that

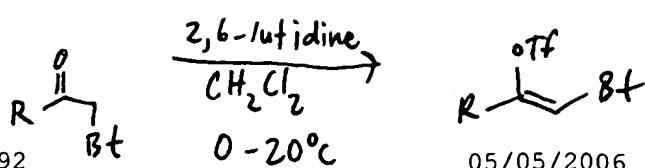
steric effects play a role and implies that these inverted, unrearranged products

are derived from in plane (σ^*) SN2 reaction. The presence of the remaining, retained, unrearranged enol triflate can be explained by a ligand coupling mechanism (π^* SN2) and the fragmentation mechanism(s) do not require the intermediacy of a primary vinyl cation.

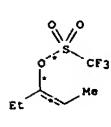
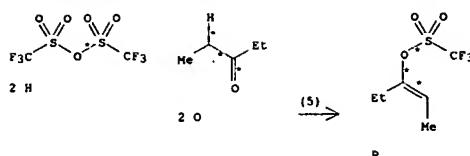
REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS

FORMAT RECORD. ALL CITATIONS AVAILABLE IN THE RE

RX(5) OF 10 2 H + 2 O ==> P + Q



L2 ANSWER 4 OF 9 CASREACT COPYRIGHT 2006 ACS on STN

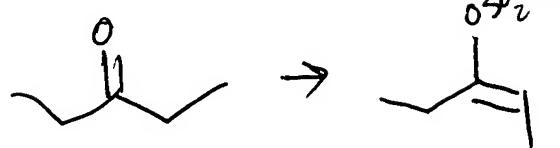


RX(5) RCT H 358-23-6, O 96-22-0

STAGE(1)
RCT L 585-48-8 2,6-Di-t-Bu-pyridine
SOL 75-09-2 CH₂Cl₂
CON 12 hours, room temperature

STAGE(2)
SOL 109-66-0 Pentane

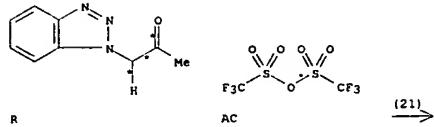
PRO P 52149-31-2, Q 52149-30-1
NTE stereoselective



L2 ANSWER 5 OF 9 CASREACT COPYRIGHT 2006 ACS on STN

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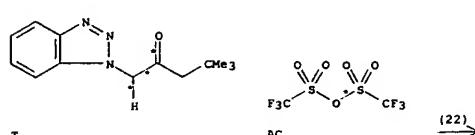
RX(21) OF 153 ...R + AC ==> AM...



AM
YIELD 88%

RX(21) RCT R 64882-50-4, AC 358-23-6
RCT AE 108-48-5 2,6-Lutidine
PRO AM 361379-21-7
SOL 75-09-2 CH₂Cl₂
NTE stereoselective

RX(22) OF 153 ...T + AC ==> AN...



L2 ANSWER 5 OF 9 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 135-257018 CASREACT

One-Carbon Homologation of Carboxylic Acids via

BtCH₂TMS: A Safe Alternative to the Arndt-Eistert

Reaction

Katritzky, Alan R.; Zhang, Suoming; Mostafa Hussein,

Abdel Heleem; Fang, Yunfeng; Steel, Peter J.

Center for Heterocyclic Compounds Department of

Chemistry, University of Florida, Gainesville, FL,

32611-7200, USA

Journal of Organic Chemistry (2001), 66 (16),

CODEN: JOCEAH; ISSN: 0022-3263

American Chemical Society

Journal

Language: English

AB Carboxylic acids are converted into the corresponding homologated acids

or esters, using easily available 1-(trimethylsilyl)methylbenzotriazole as a one-carbon synthon. The effectiveness of the reaction has been

investigated on six aryl and seven alkyl carboxylic acids.

REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR

THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

RX(20) OF 153 ...P + AC ==> AL...

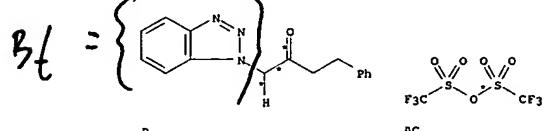


Table 1,
page 5607

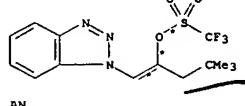
RX(20) RCT P 361379-11-6, AC 358-23-6
RCT AE 108-48-5 2,6-Lutidine



ex (g) Table 1

L2 ANSWER 5 OF 9 CASREACT COPYRIGHT 2006 ACS on STN

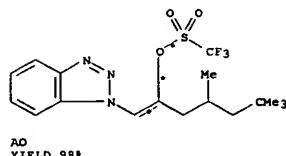
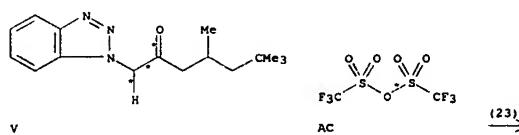
(Continued)



R = $CH_2 - C(CH_3)_3$ ex.(i)
Table 1

RX(22) RCT T 314765-22-6, AC 358-23-6
RCT AE 108-48-5 2,6-Lutidine
PRO AN 361379-22-8
SOL 75-09-2 CH₂Cl₂
NTE stereoselective

RX(23) OF 153 ...V + AC ==> AO...



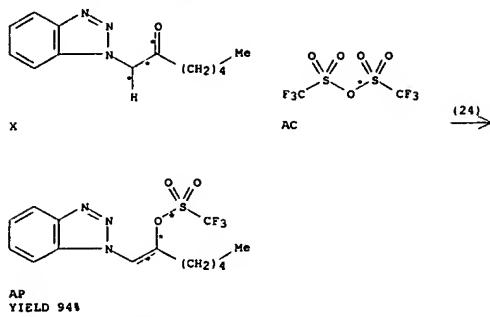
ex (j)

RX(23) RCT V 361379-13-7, AC 358-23-6
RCT AE 108-48-5 2,6-Lutidine
PRO AO 361379-23-9
SOL 75-09-2 CH₂Cl₂
NTE stereoselective

RX(24) OF 153 ...X + AC ==> AP...

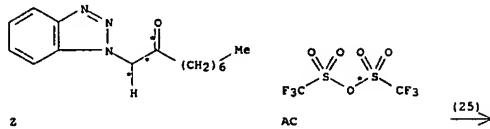
L2 ANSWER 5 OF 9 CASREACT COPYRIGHT 2006 ACS on STN

(Continued)



RX(24) RCT X 189343-44-0, AC 358-23-6
RGT AE 108-48-5 2,6-Lutidine
PRO AP 361379-24-0
SOL 75-09-2 CH2Cl2
NTE stereoselective

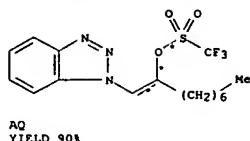
RX(25) OF 153 ...B + AC ==> AQ...



AC

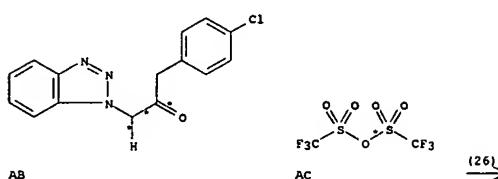
L2 ANSWER 5 OF 9 CASREACT COPYRIGHT 2006 ACS on STN

(Continued)

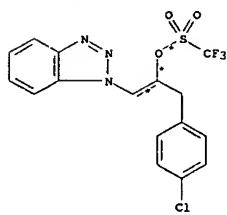


RX(25) RCT Z 304459-92-5, AC 358-23-6
RGT AE 108-48-5 2,6-Lutidine
PRO AQ 361379-25-1
SOL 75-09-2 CH2Cl2
NTE stereoselective

RX(26) OF 153 ...AB + AC ==> AR



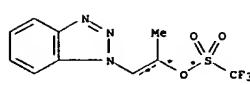
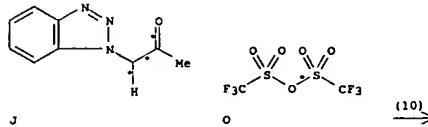
L2 ANSWER 5 OF 9 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



RX(26) RCT AB 306990-72-7, AC 358-23-6
RGT AE 108-48-5 2,6-Lutidine
PRO AR 361379-26-2
SOL 75-09-2 CH2Cl2
NTE stereoselective

L2 ANSWER 6 OF 9 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 134-71356 CASREACT
TITLE: BrCH2TMS-Assisted Homologation of Carboxylic Acids: A Safe Alternative to the Arndt-Eistert Reaction
AUTHOR(S): Katritzky, Alan R.; Zhang, Suoming; Fang, Yunfeng
CORPORATE SOURCE: Center for Heterocyclic Compounds Department of Chemistry, University of Florida, Gainesville, FL, 32611-7200, USA
SOURCE: Organic Letters (2000), 2(24), 3789-3791
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB One-carbon homologation of carboxylic acids is achieved by (i) treatment of an acyl chloride with 1-((trimethylsilylimethyl)-1H-1,2,3-benzotriazole (BrCH2TMS) to afford N-(acylmethyl)benzotriazoles, followed by (ii) conversion with triflic anhydride into RCl(OTf):CMBT, and (iii) the subsequent reaction with NaOCH3 followed by 1N HCl to afford esters RCH2CO2R' in overall yields of 50-70%. For the aliphatic compds., treatment with p-toluenesulfonic acid followed by TBAF/THF afforded acids RCH2COOH.
REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS
FORMAT RECORD. ALL CITATIONS AVAILABLE IN THE RE

RX(10) OF 69 ...J + O ==> V...



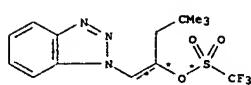
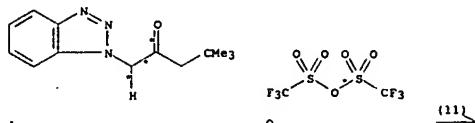
RX(10) RCT J 64882-50-4, O 358-23-6

STAGE(1)
RGT O 108-48-5 2,6-Lutidine
SOL 75-09-2 CH2Cl2

L2 ANSWER 6 OF 9 CASREACT COPYRIGHT 2006 ACS on STN (Continued)
 STAGE(2)
 SOL 110-54-3 Hexane

PRO V 314765-31-6

RX(11) OF 69 ...L + O ==> W...



RX(11) RCT L 314765-22-5, O 358-23-6

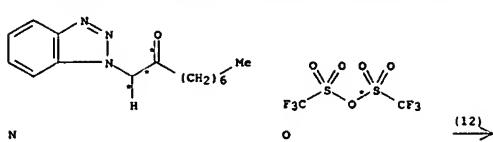
STAGE(1)
 RGT Q 108-48-5 2,6-Lutidine
 SOL 75-09-2 CH₂Cl₂

STAGE(2)
 SOL 110-54-3 Hexane

PRO W 314765-33-8

RX(12) OF 69 ...N + O ==> X...

L2 ANSWER 6 OF 9 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



RX(12) RCT N 304459-92-5, O 358-23-6

STAGE(1)
 RGT Q 108-48-5 2,6-Lutidine
 SOL 75-09-2 CH₂Cl₂

STAGE(2)
 SOL 110-54-3 Hexane
 PRO X 314765-35-0

L2 ANSWER 7 OF 9 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 106-138608 CASREACT

TITLE: Kinetics, stereochemistry, and mechanism of interaction of Vaska's complex with ethynylvinyl triflates. Formation of novel σ -butatrienyliridium compounds

AUTHOR(S): Stang, Peter J.; Dixit, Vandana; Schiavelli, Melvyn D. Drees, Paul

CORPORATE SOURCE: Dep. Chem., Univ. Utah, Salt Lake City, UT, 84112,

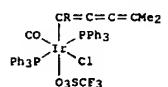
USP SOURCE: Journal of the American Chemical Society (1967), 109(4), 1150-6

CODEN: JACSAU; ISSN: 0002-7863

DOCUMENT TYPE: Journal

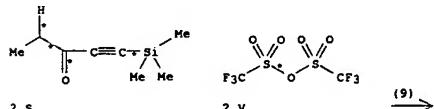
LANGUAGE: English

GI

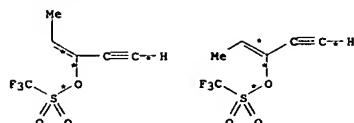


AB The reaction of Vaska's complex $[(\text{Ph}_3\text{P})_2\text{Ir}(\text{CO})(\text{Cl})]$ with $\text{Me}_2\text{C}=\text{C}(\text{O}3\text{SCF}_3)\text{C}=\text{C}\text{tbp}$ (R = H, D, Me, Ph, SiMe₃) was investigated. Oxidative addition readily occurs in benzene or toluene at room temperature to give hexacoordinate Ir(III) butatrienyl complexes I (R = same). Rate studies indicate steric inhibition by bulky substituents on the terminal acetylenic C and give high neg. entropies of activation. The reaction occurs with complete (or nearly complete) retention of olefin stereochem. A two-step SN_2' process with syn approach of the incoming Ir nucleophile is proposed to account for these observations.

RX(9) OF 28 ...2 S + 2 V ==> M + P...



L2 ANSWER 7 OF 9 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

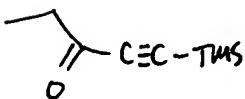


RX(9) RCT S 18387-59-1, V 358-23-6
 RGT W 38222-03-2 Me-(t-Bu)₂-2-pyridine
 PRO M 106211-71-6, P 106211-72-7
 SOL 75-09-2 CH₂Cl₂



references Synthesis, 1979, 438
 (Stang et al.)

Synthesis, 1982, 85 (105)

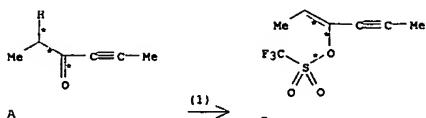


L2 ANSWER 8 OF 9 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 104-148249 CASREACT

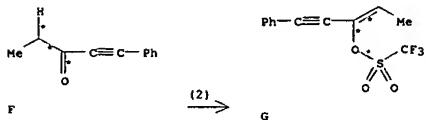
TITLE: The preparation of unsymmetrical diacetylenes from alkenylnyl triflates
AUTHOR(S): Stango, Peter J.; Dixit, Vandana
CORPORATE SOURCE: Chem. Dep., Univ. Utah, Salt Lake City, UT, 84112, USA
SOURCE: Synthesis (1985), (10), 962-3
DOCUMENT TYPE: Journal
LANGUAGE: English
AB RC.tpbond.CC(O3SCF3):CHMe (I; R = Me, Ph) were converted in 85% yield to RC.tpbond.CC.tpbond.CMe by treatment with 2,6-(Me3C)2C6H3OK in glyme. Me3SiC.tpbond.CC.tpbond.CMe was similarly prepared in 45% yield by treating I (R = Me3Si) with (Me2CH)2NLi in glyme. I were prepared by treating RC.tpbond.CC.OCOCH2Me with (CF3SO2)2O in the presence of 2,6-di-*tert*-butyl-4-methylpyridine.

RX(1) OF 9 A ==> B...



RX(1) RCT A 10575-41-6
 RGT C 38222-83-2 Me-(*t*-Bu)2-pyridine, D 358-23-6
 (F3CSO2)2O
 PRO B 101160-51-4
 SOL 75-09-2 CH2Cl2

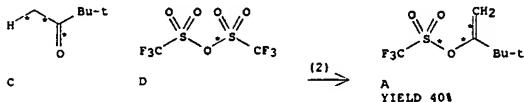
RX(2) OF 9 F ==> G...



RX(2) RCT F 19307-74-5
 RGT C 38222-83-2 Me-(*t*-Bu)2-pyridine, D 358-23-6

L2 ANSWER 9 OF 9 CASREACT COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 80-82004 CASREACT
TITLE: Vinyl triflates in synthesis. I.
tert-Butylacetylene
AUTHOR(S): Hargrove, Robert J.; Stango, Peter J.
CORPORATE SOURCE: Dep. Chem., Univ. Utah, Salt Lake City, UT, USA
SOURCE: Journal of Organic Chemistry (1974), 39(4), 581-2
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The elimination of CF3SO3H from Me3CC(O3SCF3):CH2 (I) to give MeCC.tpbond.CH is catalyzed by pyridine. Pinacolone reacts with (CF3SO2)2O to give I.

RX(2) OF 3 C + D ==> A...



RX(2) RCT C 75-97-6, D 358-23-6
 RGT E 110-86-1 Pyridine
 PRO A 27701-32-9
 SOL 56-23-5 CC14
 NTE Classification: Isomerisation; O-Sulphonation; # Conditions:
 triflic anhydride; CC14 pyridine; 15 deg 60hr

50mL of
 (c)
 0.02 mol
 & pyridine
 0.022 mol



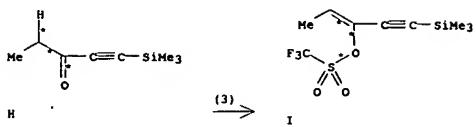
-22°C
 15min then warm to 15°C for 60hr.

add in Tf2O (0.022 mol)

L2 ANSWER 8 OF 9 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

(F3CSO2)2O
 PRO G 101160-52-5
 SOL 75-09-2 CH2Cl2

RX(3) OF 9 H ==> I...



RX(3) RCT H 18387-58-1
 RGT C 38222-83-2 Me-(*t*-Bu)2-pyridine, D 358-23-6
 (F3CSO2)2O
 PRO I 101160-53-6
 SOL 75-09-2 CH2Cl2

methods in Stango et al.

Synthesis 1979, 438

references - Dueber et al. Angew. Chem. Int. Ed. Engl. 9, 521 (1970)

1D) { Stango & Dueber, Org. Syn. 54, 79 (1974)